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PC-MODTUN & PC-FAFNIR

USER'S GUIDE

by

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1.1 Running MODTUN & FAFNIR

Seven distinct steps are required to run MODTUN and FAFNIR:

1. Do not run MODTUN or FAFNIR from within another application, such as XTGOLD or PROCOMM. Quit these applications first.
2. Create or select a run-directory
3. Make the run-directory, the current MS-DOS directory
4. Edit/create an Input Parameter File
5. Delete or rename old output (.OUT) files which may exist in the run-directory as a result of previous runs.
6. If this is a continuation run, then ensure that an Initial State File (INIT.DAT) is present.
7. Run MODTUN 1, MODTUN 2, or FAFNIR, by typing in 'MODTUN 1', 'MODTUN 2' or 'MODTUN 3' respectively.

The models use two input files: the Input Parameter File and the Initial State File. The Initial State File is optional, and is only read if the user requests it.

The names of the input and the output files are as follows:

MODPAR1.DAT	- Initial Parameter File for MODTUN 1
MODPAR2.DAT	- Initial Parameter File for MODTUN 2
MODPAR3.DAT	- Initial Parameter File for FAFNIR
INIT.DAT	- Initial State File (binary)
RESULTS.OUT	- Giant text file, containing most of the results
FINAL.OUT	- Final State file (binary)
SUMMARY.OUT	- Result summary, produced only by MODTUN 2
PARTICLE.OUT	- Particle tracking information file
ERROR.OUT	- Error message file
ECHO.OUT	- An echo of certain input parameters, produced only on request by PC-FAFNIR

INIT.DAT and FINAL.OUT have **identical** formats, so runs can be easily continued.

The format of the data files is different for each model. If final plot data generation was enabled in the Input Parameter File, then AXUM Data Sheet (.DSF) files will also be generated for each specified parameter.

1.2 Structure of the Input Parameter Files

For a complete listing of all three Input Parameter Files, see Appendix H.

- the Input Parameter File should always be edited with an ASCII editor in 'overstrike' mode.
- never insert hard tabs into an IP file
- lines should not be longer than 80 characters
- columns 1 to 19 constitute the parameter field. This is where MODTUN and FAFNIR look for the value of each parameter
- the parameter field must contain nothing but real, integer or boolean value(s)
- columns 20 to 80 constitute the comment field. Text in these columns is ignored by MODTUN and FAFNIR. Other programs, such as GRID, look for keywords in the comment field.
- numbers can be entered in free format anywhere in the parameter field
- logical parameters must appear as T (true) or F (false) on column 1

1.3 What to do if MODTUN or FAFNIR crash

The models will crash with some sort of cryptic message, from NDP-Fortran.

Input/Output related crashes usually mean:

- Corrupt or missing Input Parameter (IP) File
- Corrupt or missing Initial State File
- Can't open new output files, because older versions exist
- Can't open files because DOS has run out of new file space (handles). You are trying to run MODTUN from within another application, or, the FILES parameter is set too low in CONFIG.SYS

The source-module in which the crash occurred, can usually be found by matching the hex address of the crash, with the hex address of a module in the linker (.MAP) file, which is produced automatically by the linker.

The most likely cause of a crash is some unreasonable value or recent change in the Input Parameter File.

It is possible to build a version of MODTUN and FAFNIR which will print out the name of each subroutine as soon as it is entered. (See the -g switch and the user-debug section of the NDP Fortran-386 manual.)

1.4 Getting around power failures

At this time, only the PharLap version of MODTUN or FAFNIR can be run in power-failure-safe mode.

A very large run can be divided into up to four stages. When a power failure occurs, only the uncompleted stages are repeated. Each stage must have a separate Input Parameter File. The first stage can itself be a continuation run, with its own Initial State File. Stages 2,3 and 4 are assumed to be continuation runs of previous stages.

Input files must be placed in the following directories:

\RUNS\STAGE1 - must contain an Input Parameter File and optionally, an Initial State File (INIT.DAT)

The following three directories should either be empty, or they should contain an Input Parameter File, for continuing the run started in \RUNS\STAGE1:

\RUNS\STAGE2
\RUNS\STAGE3
\RUNS\STAGE4

After the input files are in order, the following commands can be used to start a power-failure protected run:

```
MODTUN 1 P  -  Starts MODTUN 1
MODTUN 2 P  -  Starts MODTUN 2
MODTUN 3 P  -  Starts FAFNIR
```

To conserve disk-space, output is only kept for the very last stage.

2.1 How to rebuild MODTUN and FAFNIR

Six distinct steps need to be taken:

1. Decide on the co-processor (80387 or Weitek 3167)
2. Decide on the DOS-Extender (NDP or PharLap)
3. Compile the source module(s)
4. Link the object files
5. Assign the appropriate name to the new executable file
6. Copy the new executable file to the \EXE directory

Notes for the rebuild steps:

1. Code generated for the Weitek co-processor will crash on a computer which is only equipped with an 80387 co-processor, and conversely, 80387 code will not run on a Weitek co-processor.

2. The DOS-Extender option is included for greater flexibility: the ClearView Debugger only works with the NDP DOS-Extender, on the other hand, the PharLap DOS-Extender is more reliable, and it is the only one which can be configured to run on the COMPAQ. See Appendix G for configuration details.

3. Compilation is described in Section 2.2

4. Linking is described in Section 2.3

5. After linking, the executable file will have a strange name to distinguish it from the current, working version. (See Section 2.3 for executable file names.) Current working executable files are called MODTUN1.xxx, MODTUN2.xxx, and MODTUN3.xxx, where .xxx is .LTL or .EXP depending on which DOS-Extender was used.

6. After linking, the executable file will reside in one of the following directories: \EXE\V1, \EXE\V2, or \EXE\FAFNIR. Current working versions must reside in the \EXE directory.

The last two steps can be omitted to generate a debug/test version.

2.2 How to compile MODTUN and FAFNIR source file

There are three command files in the \BATCH directory which compile **individual** modules of MODTUN and FAFNIR. These command files are called C1.BAT, C2.BAT and CF.BAT respectively. The compiler switches are hard-coded in these three files.

There are three more command files in the \BATCH directory which compile **every** module of MODTUN 1, MODTUN 2, and FAFNIR. These command files called C1ALL.BAT, C2ALL.BAT and CFALL.BAT respectively. The CxALL.BAT command files work, by making repeated calls to Cx.BAT.

To compile **every** module, use C1ALL, C2ALL, and CFALL as follows:

```
CxALL  <co-processor>  <environment>  where,
     x                -  1, 2 or F
     <co-processor>   -  INTEL or WEITEK (abbreviated I or W)
     <environment >   -  PHARLAP or NDP (abbreviated P or N)
```

To compile an **individual** module, use C1, C2, and CF as follows:

```
Cx  <module-name> <co-processor>  <environment>  where,
     x                -  1, 2 or F
     <module-name>    -  the name of the source file
     <co-processor>   -  INTEL or WEITEK (abbreviated I or W)
     <environment >   -  PHARLAP or NDP (abbreviated P or N)
```

Compilation examples:

C1ALL INTEL NDP	- compiles **every** module of MODTUN 1 for the 80387 co-processor and the NDP DOS-Extender
C1 MAIN1 W P	- compiles the MAIN1.F MODTUN 1 source-file for the Weitek co-processor and the PharLap DOS-Extender
CFALL W P	- compiles EVERY module of FAFNIR for the Weitek co-processor and the PharLap DOS-Extender
CF WRIT_ARR I P	- compiles the WRIT_ARR.F FAFNIR source file for the 80387 co-processor and the NDP DOS-Extender

The object files are all placed in a directory specific to the DOS-Extender and the co-processor. See Appendix A for details.

2.3 How to link MODTUN and FAFNIR

There are three command files in the \BATCH directory which link MODTUN 1, MODTUN 2, and PC-FAFNIR. These command files are called L1.BAT, L2.BAT and LF.BAT respectively.

To link MODTUN 1, MODTUN 2, MODTUN 3, or FAFNIR, use the L1, L2 or LF commands as follows:

Lx	<co-processor>	<environment>, where,
x	-	1, 2 or F
<co-processor>	-	INTEL or WEITEK (abbreviated I or W)
<environment >	-	PHARLAP or NDP (abbreviated P or N)

Link examples:

L1 WEITEK NDP	- link MODTUN 1 for the Weitek co-processor and the NDP DOS-Extender.
LF I P	- link FAFNIR for the Intel 80387 co-processor and the PharLap DOS-Extender

The executable files are placed in **\EXE\V1**, **\EXE\V2** or **\EXE\FAFNIR**, depending on which model was linked. The executable files will have the following names:

File Name	Model	Co-processor	DOS-Extender
INTEL1N.LTL	MODTUN 1	Intel 80387	NDP
INTEL2N.LTL	MODTUN 2	Intel 80387	NDP
INTELFN.LTL	FAFNIR	Intel 80387	NDP
INTEL1P.EXP	MODTUN 1	Intel 80387	PharLap
INTEL2P.EXP	MODTUN 2	Intel 80387	PharLap
INTELFN.EXP	FAFNIR	Intel 80387	PharLap
WEITEK1N.LTL	MODTUN 1	Weitek 3167	NDP
WEITEK2N.LTL	MODTUN 2	Weitek 3167	NDP
WEITEKFN.LTL	FAFNIR	Weitek 3167	NDP
WEITEK1P.EXP	MODTUN 1	Weitek 3167	PharLap
WEITEK2P.EXP	MODTUN 2	Weitek 3167	PharLap
WEITEKFP.EXP	FAFNIR	Weitek 3167	PharLap

2.4 How to modify existing modules

All existing modules reside in one of three source file directories:

```
\SRC\V1      - MODTUN 1 source
\SRC\V2      - MODTUN 2 source
\SRC\FAFNIR - FAFNIR source files
```

After editing an existing source file, follow the rebuild procedures outlined in Section 2.1

If you modify any include (.CMN) files, then the safest course of action is to re-compile **every** source file.

2.5 How to add a new module

The new module must be created in one of the source file directories (\SRC\V1, \SRC\V2 or \SRC\FAFNIR), after constructing the new module with an ASCII text editor, the new module's name must be inserted into **all** linker and compiler command files.

Suppose that you have just created a new source file called FRED.F for MODTUN 1, then you would have to insert references to FRED into the following files:

```
\BATCH\C1ALL.BAT     - Batch file which recompiles all of MODTUN 1
\EXE\V1\INTELP.LNK   - Linker command file for 80387/PharLap
\EXE\V1\INTELN.LNK   - Linker command file for 80387/NDP
\EXE\V1\WEITEKP.LNK - Linker command file for Weitek/PharLap
\EXE\V1\WEITEKN.LNK - Linker command file for Weitek/NDP
```

The source-file names are sorted alphabetically in all command files.

2.6 How to add a new input parameter

Twelve distinct steps are required to create a new parameter in an Input Parameter (IP) file:

1. Make a back-up copy of the current Input Parameter (IP) file in the **\RUNS\SAMPLES** directory

2. Find a spot in the IP file for the new parameter. Insert one additional line, with a comment.

3. Identify the subroutine which reads in the Input Parameter File

4. Create/make-note of the Fortran variable in which the new parameter will be stored.

5. Make sure that this variable is shared via a common-block or by passing a parameter to the read-subroutine.

6. Identify the Fortran **READ** statement which reads in existing parameters, nearest to the new parameter.

7. Modify the **READ** statement and the corresponding **FORMAT** statement, so that the new parameter will also be read.

8. Re-compile the subroutines which have been modified

9. Re-link the model whose parameter file was changed

10. Test. Use the ECHO feature with FAFNIR, or the ClearView debugger with MODTUN to make sure that the new parameter is read in correctly.

11. Back up the source files and the new Input Parameter file

12. Update the read-subroutine of the Axum Data Sheet File (.DSF) creation program corresponding to the model whose Input Parameter File was modified. (AXCONV2 or AXCONV3)

The following files contain subroutines which read the Input Parameter File:

READPARA.F - in MODTUN 1 and in MODTUN 2
READPAR1.F - in FAFNIR only
READPAR2.F - in FAFNIR and in AXCONV2
READPAR3.F - in AXCONV3 only

3.1 AXUM documentation and setup

Original documentation for AXUM consists of the following:

1. Spiral-bound AXUM user's guide
2. AXUM Release Notes 1.02 booklet, dated June 1990
3. AXUM Release Notes 1.02 booklet, dated July 1990
4. README.DOC file in the **\AXUM** directory, dated Sep 24 1990
   This is the only document which explains the use of the **gridcs()** grid-interpolation function.

AXUM uses a lot of memory, especially when 3D or contour plots are generated. AXUM will try to swap data to a disk file if there is not enough RAM memory. This feature is called **virtual memory**. The location of the swap-file can be set in **\AXUM\AXUMPATHS.DPT**. The swap-file can be on a RAMDRIVE for increased speed. The simulated disk-drive can be in extended memory. (See VDISK.SYS and RAMDRIVE.SYS in the MS-DOS 4.01 manual, and page 7 of the June 1990 AXUM release notes.)

AXUM can also use the so-called High Memory Area (HMA). This is a 64K block of memory just above 1MB. It can be accessed through an Extended Memory Manager, such as HIMEM.SYS, which is included with MS-DOS. See \AXUM\README.DOC for more details. AXUM must be explicitly instructed to use HMA, by starting it with the **AXUM -HMA** command.

Installing a virtual-disk drive and/or an Extended Memory Manager, require the following additions to the CONFIG.SYS file:

```
DEVICE=C:\DOS\HIMEM.SYS  <-- Installs the Extended Memory Manager
DEVICE=C:\DOS\RAMDRIVE.SYS 2048 /e  <-- Installs a 2MB RAM disk in
                                        extended memory
```

The presence of HIMEM.SYS can interfere with the DOS-Extenders. The DOS-Extenders may refuse to run MODTUN or FAFNIR, and complain about the lack of memory.

The following files implement re-booting for memory-intensive AXUM graphics sessions:

```
\BATCH\AXBOOT.BAT        re-boots the computer with AXCONFIG.SYS
\BATCH\NBOOT.BAT         restores the regular configuration
\AXCONFIG.SYS            CONFIG.SYS for memory-intensive AXUM
\AXAUTEX.BAT             AUTOEXEC.BAT for memory-intensive AXUM
\TOOLS\GENERAL\REBOOT.COM  re-starts the computer
```

3.2 AXUM file names

AXUM uses the following file name extensions to distinguish between different types of files:

EXTENSION	FILE TYPE
.DSF	Data Sheet File (binary and quite compact)
.GRF	Graph descriptor/parameter file
.HST	AXUM macro programming language (history) file

3.30 Creating final state plots in AXUM

Five distinct steps are required:

1. Generate AXUM-readable data (.DSF file) and run AXUM
2. Decide on the plot type
3. Load up a graph-descriptor (.GRF) file
4. For 3D spline plots, regularize the grid
5. Display the plot using the **Graph/View** or **Graph/Edit** options

Sections 3.31 to 3.34 explain steps 1 to 4.

3.31 Generating AXUM-readable data

DSF files can be generated from MODTUN 2 or FAFNIR Final State (FINAL.OUT) files. The FINAL.OUT file and the corresponding Input Parameter File (IPF) must be present in your **current** directory.

Choose the MODTUN/FAFNIR parameters which you wish to read into AXUM, by editing the Plot Data Generation section of the IPF. The **AXCONV 2, AXCONV 3** command will convert MODTUN 2 and FAFNIR IPF files respectively.

The DSF conversion programs are invoked **automatically** each time you run MODTUN or FAFNIR, but usually plot generation is disabled in the Input Parameter File, so it may be necessary to run AXCONV2 and

AXCONV3 manually.

A separate DSF file will be generated for **each** MODTUN or FAFNIR parameter which you have selected. The name of the DSF file will be the name of the FORTRAN matrix corresponding to the parameter.

AXUM assumes that DSF files reside in the \AXUM\DATA directory. This default can changed in the **Setup/Paths** menu.

3.32 Final State plot types

There are three basic plot types: 2D Axial Profile, 2D Radial Profile, 3D Spline.

Axial profile is taken at a fixed radial grid line, and conversely, radial profile is taken at a fixed axial grid line.

3D Spline produces a smoothed/interpolated surface over a regularized grid.

A fourth type of plot, 3D Surface Irregular, can be used to inspect the raw data, without any interpolation.

3.33 Final State Graph Descriptor files

Sample 2D and 3D graph-descriptor (GRF) files exist in the \AXUM\GRAPH directory. Press the **Insert** key in the Graph/File/Load menu, to get a list the currently available GRF files.

2D Axial Profile samples have names such as **U15AX.GRF** (U-velocity axial profile at radial grid line #15)

2D Radial Profile samples have names such as **T1RAD.GRF** (Temperature radial profile at axial grid line #1)

3D samples have names such as **W3D.GRF** (W-velocity 3D plot)

3.34 Regularizing the grid for 3D Spline plots

The AXUM macro programs which perform the necessary interpolation are called U3D.HST, V3D.HST etc. Press the **Insert** key in the Data/History/Editor/Load menu to get a list of the available 3D history (program) files.

Always exercise the Data/History/Editor/Clear option **before** loading up a 3D (or any) program.

The only real difference between the 3D programs is the name, and the path to the DSF file which they manipulate.

Each 3D program begins with the following comment/declaration section:

```
/*****************************************************************************
  1. A full path name may need to be be specified for the .DSF file.
  2. The range of columns in the CopyCol command must extend to the
     last axial grid line. [ ie {T002R..T088R} if there were 88 axial
     grid lines in the simulation.
  3. 3-D zooming can be performed by changing minx,maxx,miny,maxy.
  4. Autoscaling is used if min=max.
  5. The max dimension of the regularized output grid is 128 x 128.
  6. The 3-D surface can be made smoother by increasing xSmooth, ySmooth.
*****************************************************************************/

LoadDS P.DSF, DataSheet = P;
CopyCol {P002R..P031R} to DataSheet = C3DTEMP, {2};

nx_out  = 55;  /* Number of axial grid lines in the regularized grid     */
ny_out  = 55;  /* Number of radial grid lines in the regularized grid    */
minx_out= 0.0; /* Lower bound of the axial grid  +---------------------+ */
maxx_out= 0.0; /* Upper bound of the axial grid  ! If min = max, then  ! */
miny_out= 0.0; /* Lower bound of the radial grid ! autoscaling is used ! */
maxy_out= 0.0; /* Upper bound of the radial grid +---------------------+ */
xSmooth = 1;   /* Degree of smoothness in the axial direction  1 normal  */
ySmooth = 1;   /* Degree of smoothness in the radial direction 2,3, high */
```

After running a 3D program, you can experiment with the interpolation parameters listed above, by running the **REGRID** program. REGRID has the same adjustable interpolation parameters as the 3D programs.

The results of the interpolation will always be stored in 3 output columns called XOUT, YOUT and ZOUT. To generate 3D Surface Irregular plots, use the **raw** data in columns X, Y and Z.

Appendix A1 MODTUN & FAFNIR directories and files

\NDPF310	NDP Fortran-386 compiler, NDP Tools, ClearView
\PHARLAP	The PharLap Tools
\RUNS\SAMPLES	Sample copies of the Input Parameter Files
\RUNS\STAGE1	Used by power-failure safe runs of MODTUN & FAFNIR
\RUNS\STAGE2	Used by power-failure safe runs of MODTUN & FAFNIR
\RUNS\STAGE3	Used by power-failure safe runs of MODTUN & FAFNIR
\RUNS\STAGE4	Used by power-failure safe runs of MODTUN & FAFNIR
\SRC\FAFNIR	FAFNIR source files
\SRC\V1	MODTUN 1 source files
\SRC\V2	MODTUN 2 source files
\OBJ\NDP	object files generated for the NDP environment with the NDP (.EXE or .LTL) version of the NDP Fortran-386 compiler
\OBJ\PHARLAP	object files generated for the PharLap environment with the PharLap (.EXP) version of the NDP Fortran-386 compiler

In the following descriptions, '...' stands for either \OBJ\NDP or \OBJ\PHARLAP.

...\V1\INTEL	contains MODTUN 1 80387 object code
...\V1\WEITEK	contains MODTUN 1 Weitek object code
...\V2\INTEL	contains MODTUN 2 80387 object code
...\V2\WEITEK	contains MODTUN 2 Weitek object code
...\FAFNIR\INTEL	contains FAFNIR 80387 object code
...\FAFNIR\WEITEK	contains FAFNIR Weitek object code

The following batch (.BAT) files make compiling and linking MODTUN and FAFNIR painless. Their usage is explained in Section 2.

\BATCH\CFALL.BAT	recompiles every FAFNIR source file
\BATCH\C1ALL.BAT	recompiles every MODTUN 1 source file
\BATCH\C2ALL.BAT	recompiles every MODTUN 2 source file
\BATCH\C1.BAT	recompiles one MODTUN 1 source file
\BATCH\C2.BAT	recompiles one MODTUN 2 source file
\BATCH\CF.BAT	recompiles one MODTUN 2 source file
\BATCH\L1.BAT	links PC-MODTUN version 1
\BATCH\L2.BAT	links PC-MODTUN version 2
\BATCH\LF.BAT	links PC-FAFNIR
\BATCH\MODTUN.BAT	runs MODTUN or FAFNIR
\EXE\FAFNIR	FAFNIR linker command, map and executable files
\EXE\V1	MODTUN 1, linker command, map and exe files
\EXE\V2	MODTUN 2, linker command, map and exe files

The three EXE directories **each** contain four linker command files:

INTELP.LNK	links 80387 code in the PharLap environment
INTELN.LNK	links 80387 code in the NDP environment
WEITEKP.LNK	links Weitek code in the PharLap environment
WEITEKN.LNK	links Weitek code in the NDP environment

The following two files implement power-failure protection:

\POWER.BAT
\BATCH\POWER2.BAT

Appendix A2 AXUM graphics directories and files

\BATCH\AXCONV.BAT runs the DSF conversion programs

\EXE\AXCONV	programs to convert Final State Files into AXUM loadable .DSF (Data Sheet File) format
\OBJ\AXCONV2	object files
\OBJ\AXCONV3	object files
\SRC\AXCONV2	Source code for MODTUN 2 Final State File conversion
\SRC\AXCONV3	Source code for MODTUN 3 Final State File conversion

The two source directories also contain the batch files which re-compile and re-link AXCONV2 and AXCONV3.

The following files implement re-booting for memory-intensive AXUM graphics sessions:

\BATCH\AXBOOT.BAT	re-boots the computer with AXCONFIG.SYS
\BATCH\NBOOT.BAT	restores the regular configuration
\AXCONFIG.SYS	CONFIG.SYS for memory-intensive AXUM
\AXAUTEX.BAT	AUTOEXEC.BAT for memory-intensive AXUM
\TOOLS\GENERAL\REBOOT.COM	re-starts the computer

Appendix B Compiler and Linker switches

The three batch files (C1.BAT, C2.BAT, CF.BAT) which compile individual modules, contain all the NDP Fortran-386 compiler switches.

At this time, the following compiler switches are in use:

For Intel 80387 code: **-n2 -n3**
For Weitek 3167 code: **-n4 -n6 -n7 -n8**

In addition, FAFNIR modules are optimized with the **-O -on** switches, and the **ISWEEPF.F** FAFNIR module is still further optimized with the

-OL switch. (See \OBJ\PHARLAP\FAFNIR\WEITEK\README.DOC file for more details.)

For a full description of all compiler switches, consult the NDP Fortran-386 User's Manual.

The linker command files INTELP.LNK, INTELN.LNK, WEITEKP.LNK, and WEITEKN.LNK contain all the linker switches. There are **three sets** of these linker command files, one for each model.

The first three modules of any linker command file **must** be the following, in this order:

1. \NDPF310\DOS386.OBJ - NDP interface to DOS Extender
2. \NDPF310\co-processor module
3. \NDPF310\PROFDUMY.OBJ
4. The MAIN module (for NDP linker only)

The co-processor module is __CO387.OBJ for the Intel 80387, co-processor, or __CO1167.OBJ for the Weitek 3167 co-processor.

Libraries must also be specified in the linker command files. The order and the name of the libraries depends on the co-processor and the DOS-Extender. See \EXE\FAFNIR*.LNK for examples.

Appendix C Differences between VAX-Fortran and NDP Fortran-386

The functions and subroutines which return the time and date are quite different in the two environments.

SECNDS is an integer function which takes an integer argument in NDP Fortran, and it is a real function with a real argument in VAX (and Unix) Fortran. In NDP Fortran, **SECNDS** must be declared integer in each module where its used.

There is no function corresponding to NDP-Fortran's DOSTIM. DOSTIM is used in one module (PRINT_TI.F) of all three models. DOSTIM can, of course, be implemented in VAX-Fortran.

In order to avoid numeric exceptions in the VAX/VMS environment, it may be necessary to start the VAX versions of these models with the following code:

```
C
C     Continue on overflows and underflows
C
CALL ERRSET(70,.TRUE.,.FALSE.,.FALSE.,.FALSE.)  ! Integer overflow
CALL ERRSET(71,.TRUE.,.FALSE.,.FALSE.,.FALSE.)  ! Integer zero divide
CALL ERRSET(72,.TRUE.,.FALSE.,.FALSE.,.FALSE.)  ! Floating overflow
CALL ERRSET(73,.TRUE.,.FALSE.,.FALSE.,.FALSE.)  ! Floating zero divide
CALL ERRSET(74,.TRUE.,.FALSE.,.FALSE.,.FALSE.)  ! Floating underflow
```

Appendix D Background note on NDP Tools and the PharLap Tools

NDP Tools and the PharLap Tools both contain a utility called a DOS-Extender. The DOS-Extender is a program which can load and execute very large programs. The NDP DOS-Extender is called NDPRUN.EXE, and the PharLap DOS-Extender is called RUN386.EXE. The two DOS-Extenders have many similarities and differences. The major difference is that each DOS-Extender is only capable of running one specific type of executable file.

PharLap compatible programs have the extension .EXP, and NDP compatible programs have the extension .LTL

The NDP Fortran-386 compiler is capable of generating object code for both DOS-Extenders. NDP-Fortran also includes two different set of libraries, one is made for the PharLap environment, the other is made for the NDP Environment.

The following compilation examples illustrate how to build PharLap and NDP compatible programs, using MicroWay's **compiler-driver, mf77**. It is assumed that NDP-Fortran is installed in the **\NDP** directory, and the PharLap Tools are installed in the **\PHARLAP** directory, and that both of these directories are in the current search PATH.

NDP DOS-Extender compilation example:

```
SET NDP  = \NDP
SET LIBP = \NDP\LIB
SET TOOLS= \NDP

mf77 -n2 test.f  <-- Generates TEST.LTL utilizing the 80387
mf77 -n4 test.f  <-- Generates TEST.LTL utilizing the Weitek
ndprun test      <-- Runs TEST.LTL
```

PharLap DOS-Extender compilation example:

```
SET NDP  = \NDP
SET LIBP = \NDP\LIB
SET TOOLS= \PHARLAP

mf77 -n2 -asm -exp test.f  <--- Generates TEST.EXP for the
                               80387 co-processor
mf77 -n4 -asm -exp test.f  <--- Generates TEST.EXP for the
                               Weitek co-processor
run386 test                <--- Runs TEST.EXP
```

Currently, PC-MODTUN and PC-FAFNIR are built for the PharLap environment. The PharLap DOS-Extender and the PharLap Linker are more reliable than their NDP counterparts. However, NDP Fortran may have less PharLap support in the future, so the next revision of PC-MODTUN and PC-FAFNIR will be built in the NDP environment.

Appendix E Software Tool Revision Numbers and Release Dates

Software Tools Used
NDP Tools Version 3.0
NDP Fortran-386 Version 3.1.0 for NDP Tools
NDP Fortran-386 Version 3.1.0 for PharLap Tools
NDP C-386 Version 3.1.0
ClearView Debugger Version 1.1a for DOS
PharLap Tools Version 2.2d
AXUM Graphics Version 1.02 Sept. 24 1990 release

The following files are newer, beta-test **replacements** **currently in use**.

NAME	DESCRIPTION	SIZE	DATE
NDPF386.EXE	Fortran compiler program	871935	Jan 31 1991
NDPLINK.EXE	Linker program	255061	Mar 14 1991
DOS386.EXE	Key NDP module	11118	Jan 08 1991

MicroWay is notorious for relying on their customers to debug their products. The revision and the date of MicroWay tools should be carefully noted. For example, the linker which is included with NDP Tools Version 3.0, can't link programs which have more than a couple of hundred subroutines, a later beta-test version is superior.

Friendly technical support is available at the following telephone numbers:

NDP Fortran MicroWay Inc. (508)746-7341 user# 103956
AXUM Graphics TriMetrix Inc. (206)527-9912 serial# AX-010-12131

Appendix F Recommended backup regime

Use the PKZIP compression/backup tool from PKWARE Inc. PKZIP is built into the XTGOLD 2.0 hard disk browser.

At the end of **each** programming session:

1. Run XTGOLD. Change the sort order to descending by date.
2. **Tag** all changed files. (Source, batch, linker-command, Input Parameter etc.)
3. Turn on SHOWALL
4. Create a new zip file using today's date as its name. For example 91JUL18.ZIP . Multiple backup sets on the same day can be distinguished by the suffix A,B,C etc. For example: 91JUL20A.ZIP, 91JUL20B.ZIP etc.

This procedure will create incremental backups. From time to time, make a PKZIP backup of **all** files for each model.

Currently, backups made by Atlantis Scientific, are on two 3.5 in floppy diskettes, labelled "FAFNIR/AXUMIO BACKUPS", and "MODTUN SOURCE FILES BACKUP V1 V2". There are 3 copies of each diskette. Copy #3 is at Atlantis Scientific's offices.

Appendix G Differences between the ALR and the COMPAQ environments

ALR

- The ALR is equipped with a Weitek 3167 and an Intel 80387
- All directories, files and software tools which are required to develop MODTUN & FAFNIR are installed.
- Both DOS-Extenders (NDP & PharLap) run on the ALR computer without any special switches.

COMPAQ

- The COMPAQ computer **does not** have a Weitek co-processor, it is equipped with an Intel 80387 co-processor only.
- Only the latest executable files for MODTUN and FAFNIR are installed.
- The name of the directories where MODTUN, FAFNIR and the DOS-Extenders reside are different in the COMPAQ than in the ALR.
- The 80386 CPU currently in the motherboard has the so called **paging bug.**
- Only the PharLap DOS-Extender can work around the paging bug.
- The PharLap DOS-Extender requires the following switches to operate correctly: -NOPAGE -CEMM -B0 -1167 OFF
- The PharLap DOS-Extender **has been** pre-configured with the required switches, using PharLap's CFIG386 utility.

Appendix H MODTUN 1 Input Parameter File

```
+------------------------------------------------------------- Version 1.1 ----+
!                      MODTUN Input Parameter File                             !
+------------------------------------------------------------------------------+
C1
C2
C3                  Sample MODTUN 1 Input Parameter File
C4
C5
C6
C7                   Recent additions: XDIST, TADIAB
C8
C9
+------------------------------------------------------------- Version 1.1 ----+
!         Parameters To Control Execution Of Current Run                       !
+------------------------------------------------------------------------------+
1                   IRUN    current run number
100                 MAXIT   number of iterations in current run
100                 INDPRI  full output every this many iterations
12                  IMON    I index of monitoring station for output
12                  JMON    J index of monitoring station for output
1.0E-10             SORMAX  max. sum of sources
+------------------------------------------------------------- Version 1.1 ----+
!              Parameters To Control Convergence                               !
+------------------------------------------------------------------------------+
2                   NSWPU   # of sweeps for U
2                   NSWPV           "       V
1                   NSWPP           "       P
1                   NSWPK           "       K
1                   NSWPD           "       D
1                   NSWPX           "       X
1                   NSWPH           "       H
5                   NSWPRA          "       RA
1                   NSWPCO          "       CO
1                   NSWPW           "       W
0.6                 URFU    under relaxation factor for U
0.6                 URFV                    "       V
1.0                 URFP                    "       P
0.6                 URFE                    "       E
0.6                 URFK                    "       K
1.0                 URFVIS                  "       VIS
0.6                 URFCO                   "       CO
0.6                 URFX                    "       X
0.2                 URFVOL                  "       VOL
0.6                 URFPR                   "       PR
0.6                 URFH                    "       H
1.0                 URFRAD                  "       RAD
0.6                 URRRCO                  "       RCO
0.6                 URFW                    "       W
+------------------------------------------------------------- Version 1.1 -+
!    Logical Parameters To Control What Is Calculated And Output             !
+-----------------------------------------------------------------------------+
T                   T - combustion run, F - isothermal run
F                   Default Entrance Velocity Profiles
T                   Default axial/radial grid
T                   Default Turbulent Kinetic Energy Entrance Profile
T                   Default Dissipation Entrance Profile
T                   Create a Results Summary File [ Specify contents on the 2nd
T                   INCALU                          column of the plot selection
T                   INCALV                          lines. See farther down. ]
T                   INCALP
T                   INCALK
T                   INCALD
T                   INPRO
T                   IFLOW
T                   INTRAK
T                   IPISO
```

```
T                 IADBWL
F                 INCACO
T                 INCALT
T                 INCALH
T                 INCALX
T                 INCARD
T                 INCAPR
T                 INCALW
T                 IQUARL
F                 ICONE
F                 ISWRW
T                 LOWVOL
F                 NOSLIP
0.035             XDIST(1) interpolate & print field values here at the end
0.125             XDIST(2) interpolate & print field values here at the end
0.205             XDIST(3) interpolate & print field values here at the end
0.3472            XDIST(4) interpolate & print field values here at the end
0.42              XDIST(5) interpolate & print field values here at the end
1.27              XDIST(6) interpolate & print field values here at the end
+------------------------------------------------------- Version 1.1 -----+
!                 Coal Related Quantities                                 !
+-----------------------------------------------------------------------+
0.1261            FASH  % of ash in coal
0.3903            FRESC % of C in coal
0.3798            FVOLC % of volatiles in coal
0.0401            FHY   % of H2 in coal
0.0032            FSU   % of S in coal
0.0127            FN2   % of N2 in coal
0.0478            FOX   % of O2 in coal
0.0               FMH2O  mass fraction of H2O in coal
328.08E+05        CALVAL calorific value of carbon
922.0E+04         CALVCO calorific value of CO
30.               B1111  rate constant for devolatilization
0.090909          ZL     ratio of mass flow of coal to masflo of air
1200.             DENP   initial density of particles in kg/m**3
2.93E+07          SIG    Std Dev of Activ Engy for High Vol Devol
2.12E+08          EO     Activ Engy for High Vol Devol
1.67E+13          FKO    Pre-expon Fctr for High Vol Devol
0.65E+08          ACTES  Activ Engy for Low Vol Devol
0.35              PSII2  For Calc Pre-expon Fctr Low Vol Devol
1.015E+08         ACTE   Activ Engy for Char Burn
0.8596            AF     Pre-expon Fctr for High Vol Char Burn
8.5               ACOMB  Used in Volatile Combustion (=A)
2.0               BCOMB  Used in Volatile Combustion (=A')
0.008             SII1   Used in calc of AKCH for Low Vol Char Burn
0.01              SII2   Used in calc of AKCH for Low Vol Char Burn
0.0001            SII3   Used in calc of AKCH for Low Vol Char Burn
0.4               XRN    Used in calc of AKCH for Low Vol Char Burn
+------------------------------------------------------- Version 1.1 ---+
!               Particle Tracking Input Information                     !
+-----------------------------------------------------------------------+
4                 NPS    # of particle sizes to be tracked
4.0E-05           PD(1)   particle diameter
6.0E-05           PD(2)
8.75E-05          PD(3)
1.25E-04          PD(4)
1.0E-04           PD(5)
1.0E-04           PD(6)
1.0E-04           PD(7)
4                 NSL     # of loc. of the particle start considered
0.01              YST(1)  distance of firing location of particle
0.019             YST(2)  from center in m
0.029             YST(3)
0.038             YST(4)
13.0              UPST(1) particle start velocity in m/s
13.27             UPST(2)
10.77             UPST(3)
6.53              UPST(4)
0.11              FRACT(1) fraction of particles in particle size
```

```
0.63              FRACT(2)
0.16              FRACT(3)
0.1               FRACT(4)
0.0               FRACT(5)
0.0               FRACT(6)
0.0               FRACT(7)
+------------------------------------------------------------ Version 1.1 -->+
!              Parameters Describing Plot File                               !
+------------------------------------------------------------------------------+
1                 Horiz. plot-grid start
51                Horiz. plot-grid end
1                 Vertical plot-grid start
37                Vertical plot-grid end
5                 Frequency of iterations to save for plotting
T                 Save some of the following fields for plotting
T  T              U velocity - u(i,j)      [ 1st col. Plot, 2nd column Summary ]
F  T              V velocity - v(i,j)
T  T              W velocity - w(i,j)
F  F              Pressure - p(i,j)
T  F              Turbulence Energy - te(i,j)
T  F              Energy dissipation rate - ed(i,j)
F  F              Effective viscosity - vis(i,j)
F  F              Mass source into gas phase - spm(i,j)
T  F              Unburnt coal passing through - colmas(i,j)
F  F              Enthalpy source into gas phase - sph(i,j)
F  F              Oxygen source into gas phase - spox(i,j)
F  F              Volatile source into gas phase - spf01(i,j)
F  F              CO source into gas phase - spco(i,j)
F  F              CO2 source into gas phase - spf02(i,j)
T  F              Mass fraction of oxygen - amox(i,j)
T  F              Mass fraction of volatiles - f01(i,j)
F  F              Mass fraction of CO - co(i,j)
T  F              Mass fraction of CO2 - f02(i,j)
T  T              (Particle temperature)**4 - stp4(i,j)
F  F              SKP (=projtd part area/unit vol.)- skp(i,j)
T  F              Radiation source in enthalpy - surad(i,j)
F  F              (Radiation temperature)**4 - tr4(i,j)
F  F              Enthalpy - h(i,j)
T  T              Temperature deg.K - t(i,j)
F  F              Density of fluid - den(i,j)
+------------------------------------------------------------ Version 1.1 -->+
!             Parameters Describing Air Input                                !
+------------------------------------------------------------------------------+
1.176             DENSIT density of air at 300 deg.K
3.6E-05           VISCOS dynamic viscosity of air at 300K in kg/ms
1.036             SWN    swirl number
9.6877            UIN    U velocity at inlet of domain in m/s
0.049443          PAFIN  primary air flow kg/s
0.133279          SAFIN  secondary air flow kg/s
318.16            TAIRP  primary air temperature in deg. K
307.16            TAIRS  secondary air temperature in deg. K
0.02              C11    constant for turbulence in KE model
1000.0            TEMPIN initial gas field temperature in deg. K
+------------------------------------------------------------ Version 1.1 -->+
!              Entrance Velocity Profiles                                    !
+------------------------------------------------------------------------------+
0.0               U(2,1) Initial U velocity. U(2,1),U(2,2),U(2,3),...
12.02             U(2,2)
12.65             U(2,3)
13.32             U(2,4)
13.12             U(2,5)
11.19             U(2,6)
8.52              U(2,7)
6.53              U(2,8)
4.82              U(2,9)
2.37              U(2,10)
5.77              U(2,11)
11.47             U(2,12)
14.78             U(2,13)
```

```
-9999           End of U-velocity data
0.0             V(1,1) Initial V velocity. V(1,1),V(1,2),V(1,3),...
0.86            V(1,2)
1.0             V(1,3)
1.31            V(1,4)
1.62            V(1,5)
1.94            V(1,6)
1.91            V(1,7)
1.71            V(1,8)
1.46            V(1,9)
1.47            V(1,10)
0.08            V(1,11)
0.52            V(1,12)
2.5             V(1,13)
-9999           End of V-velocity data
0.0             W(1,1) Initial W velocity. W(1,1),W(1,2),W(1,3),...
0.0             W(1,2)
0.0             W(1,3)
0.0             W(1,4)
0.0             W(1,5)
0.0             W(1,6)
0.04            W(1,7)
0.32            W(1,8)
0.49            W(1,9)
0.81            W(1,10)
10.08           W(1,11)
16.44           W(1,12)
16.12           W(1,13)
-9999           End of W-velocity data
+------------------------------------------------------------- Version 1.1 -+
!                Turbulent Kinetic Energy Entrance Profile                  !
+---------------------------------------------------------------------------+
0.0             TE(1,1)
-9999           End of Turbulent Kinetic Energy Entrance Profile data
+------------------------------------------------------------- Version 1.1 -+
!                Dissipation Entrance Profile                               !
+---------------------------------------------------------------------------+
0.0             ED(1,1)
-9999           End of Dissipation Entrance Profile data
+------------------------------------------------------------- Version 1.1 -+
!                      Geometry Of Furnace                                  !
+---------------------------------------------------------------------------+
2               ISTEP   I index of entrance plane
3               JSTEP   J index of entrance plane
51              NI      max. value of I index
37              NJ      max. value of J index
51              IT      max. value of I index
37              JT      max. value of J index
29              JOUT    location of furnace exit radius
32              IADIAB  location of end of adiabatic wall
410.0           TWALL   wall temp. AFTER the adiabatic section
-9999           TADIAB  wall temp. IN the adiab. section (-9999=use default)
1               J1STP   geometry of burner
10              J2STP
10              J3STP
13              J4STP
15              J5STP
34              J6STP
0.49            RLARGE  radius of tunnel furnace in meters
5.37            ALTOT
15              ISTEPS  Start of Quarl
24              ISTEPE  End of Quarl
25              JSTEPE
+------------------------------------------------------------- Version 1.1 -+
!                        X-Y Grid Locations                                 !
+---------------------------------------------------------------------------+
-0.005          X(1)     Axial grid coordinates X(1),...,X(51)
0.005           X(2)
0.016           X(3)
```

```
0.028           X(4)
0.041           X(5)
0.055           X(6)
0.07            X(7)
0.086           X(8)
0.103           X(9)
0.12            X(10)
0.1334          X(11)
0.1534          X(12)
0.1734          X(13)
0.1934          X(14)
0.2144          X(15)
0.2324          X(16)
0.2534          X(17)
0.2734          X(18)
0.2934          X(19)
0.3134          X(20)
0.3334          X(21)
0.3534          X(22)
0.3734          X(23)
0.3934          X(24)
0.4134          X(25)
0.4291          X(26)
0.49            X(27)
0.55            X(28)
0.61            X(29)
0.67            X(30)
0.73            X(31)
0.8             X(32)
0.9             X(33)
1.0             X(34)
1.1             X(35)
1.2             X(36)
1.33            X(37)
1.476           X(38)
1.636           X(39)
1.814           X(40)
2.0             X(41)
2.23            X(42)
2.47            X(43)
2.74            X(44)
3.04            X(45)
3.37            X(46)
3.74            X(47)
4.15            X(48)
4.6             X(49)
5.1             X(50)
5.64            X(51)
-0.002          Y(1)   Radial grid coordinates  Y(1),...,Y(37)
0.002           Y(2)
0.0085          Y(3)
0.015           Y(4)
0.0216          Y(5)
0.0281          Y(6)
0.0346          Y(7)
0.0411          Y(8)
0.0453          Y(9)
0.05            Y(10)
0.0573          Y(11)
0.0667          Y(12)
00.073          Y(13)
0.0794          Y(14)
0.0879          Y(15)
0.0963          Y(16)
0.1061          Y(17)
0.1154          Y(18)
0.1248          Y(19)
0.1341          Y(20)
0.1437          Y(21)
```

```
0.1527              Y(22)
0.1621              Y(23)
0.1714              Y(24)
0.1807              Y(25)
0.188               Y(26)
0.2065              Y(27)
0.2268              Y(28)
0.249               Y(29)
0.2735              Y(30)
0.3004              Y(31)
0.3299              Y(32)
0.3623              Y(33)
0.397               Y(34)
0.437               Y(35)
0.4738              Y(36)
0.5105              Y(37)
+------------------------------------------------------------ Version 1.1 --------+
!                  End of the MODTUN Input Parameter File                          !
+--------------------------------------------------------------------------------+
```

Appendix I MODTUN 2 Input Parameter File

```
+------------------------------------------------------------------ Version 2.0 ----+
!                        MODTUN Input Parameter File                                !
+-------------------------------------------------------------------------------+
C1
C2                  Sample MODTUN 2 Input Parameter File
C3
C4
C5
C6
C7 Version 2.0 MODTUN; IEA Test Case; grid as stated; single reaction model;
C8 devol param as stated; char comb pre-exponential param mid value;
C9 1700 its isothermal; 7000 its comb.; + 3000 its comb;more info on particle 7
+------------------------------------------------------------------ Version 2.0 ---+
!          Parameters To Control Execution Of Current Run                          !
+-------------------------------------------------------------------------------+
3                   IRUN    current run number
3000                MAXIT   number of iterations in current run
3000                INDPRI  full output every this many iterations
12                  IMON    I index of monitoring station for output
12                  JMON    J index of monitoring station for output
1.0E-10             SORMAX  max. sum of sources
+------------------------------------------------------------------ Version 2.0 ---+
!                Parameters To Control Convergence                                 !
+-------------------------------------------------------------------------------+
2                   NSWPU   # of sweeps for U
2                   NSWPV           "       V
1                   NSWPP           "       P
1                   NSWPK           "       K
1                   NSWPD           "       D
1                   NSWPX           "       X
1                   NSWPH           "       H
5                   NSWPRA          "       RA
1                   NSWPCO          "       CO
1                   NSWPW           "       W
0.6                 URFU    under relaxation factor for U
0.6                 URFV                    "           V
1.0                 URFP                    "           P
0.6                 URFE                    "           E
0.6                 URFK                    "           K
1.0                 URFVIS                  "           VIS
0.6                 URFCO                   "           CO
0.6                 URFX                    "           X
0.2                 URFVOL                  "           VOL
0.6                 URFPR                   "           PR
0.6                 URFH                    "           H
1.0                 URFRAD                  "           RAD
0.6                 URRRCO                  "           RCO
0.6                 URFW                    "           W
+------------------------------------------------------------------ Version 2.0 -+
!    Logical Parameters To Control What Is Calculated And Output                    !
+-------------------------------------------------------------------------------+
T                   T - combustion run, F - isothermal run
Single Reaction     Model: Two Competing, Multiple Parallel, Single Reaction
F                   Default Entrance Velocity Profiles
F                   Default axial/radial grid
F                   Default Turbulent Kinetic Energy Entrance Profile
F                   Default Dissipation Entrance Profile
T                   Default (hardcoded) initial temperature field
T                   Create a Results Summary File [ Specify contents on the 2nd
T                   INCALU                          column of the plot selection
T                   INCALV                          lines. See farther down. ]
T                   INCALP
T                   INCALK
T                   INCALD
T                   INPRO
T                   IFLOW
```

```
T                INTRAK
T                IPISO
T                IADBWL
F                INCACO
T                INCALT
T                INCALH
T                INCALX
T                INCARD
T                INCAPR
T                INCALW
F                IQUARL
F                ICONE
F                ISWRW
F                LOWVOL
F                NOSLIP
0.910            XDIST(1) Tg & Conc O2 & CO2 profls @ XDIST in results & smry
1.24             XDIST(2)     "              "              "
1.39             XDIST(3)     "              "              "
2.14             XDIST(4)     "              "              "
2.29             XDIST(5)     "              "              "
3.35             XDIST(6)     "              "              "
+------------------------------------------------------------ Version 2.0 -----+
!                Coal Related Quantities                                       !
+------------------------------------------------------------------------------+
0.1110           FASH  % of ash in coal
0.4739           FRESC % of C in coal
0.2138           FVOLC % of volatiles if coal
0.0379           FHY   % of H2 in coal
0.0026           FSU   % of S in coal
0.0093           FN2   % of N2 in coal
0.1515           FOX   % of O2 in coal
0.0              FMH2O  mass fraction of H2O in coal
328.08E+05       CALVAL calorific value of carbon
922.0E+04        CALVCO calorific value of CO
30.              B1111  rate constant for devolatilization
0.136994         ZL     ratio of mass flow of coal to masflo of prim. air
1200.            DENP   initial density of particles in kg/m**3
2.93E+07         SIG    Std Dev of Activ Engy for High Vol Devol
2.12E+08         EO     Activ Engy for High Vol Devol
1.67E+13         FKO    Pre-expon Fctr for High Vol Devol
0.494E+08        ACTES  Activ Engy for Low Vol Devol
7.295E-02        PSII   For calculating the pre-expon factor of AKCH
2.392            PSII2  For Calc Pre-expon Fctr Low Vol Devol
7.1E+07          ACTE   Activ Engy for Char Burn
0.8596           AF     Pre-expon Fctr for High Vol Char Burn
6.0              ACOMB  Used in Volatile Combustion (=A)
2.0              BCOMB  Used in Volatile Combustion (=A')
+------------------------------------------------------------ Version 2.0 ---+
!              Particle Tracking Input Information                             !
+------------------------------------------------------------------------------+
4                NPS    # of particle sizes to be tracked
7                NNPP   More info on this particl?
1.2E-05          PD(1)   particle diameter
3.8E-05          PD(2)
6.2E-05          PD(3)
8.8E-05          PD(4)
1.0E-04          PD(5)
1.0E-04          PD(6)
1.0E-04          PD(7)
4                NSL     # of loc. of the particle start considered
0.0100           YST(1)  distance of firing location of particle
0.0190           YST(2)  from center in m
0.0290           YST(3)
0.038            YST(4)
28.94            UPST(1) particle start velocity in m/s
29.15            UPST(2)
22.33            UPST(3)
12.46            UPST(4)
0.180            FRACT(1) fraction of particles in particle size
```

```
0.250              FRACT(2)
0.210              FRACT(3)
0.360              FRACT(4)
0.0                FRACT(5)
0.0                FRACT(6)
0.0                FRACT(7)
+------------------------------------------------------------ Version 2.0 --+
!            Parameters Describing Plot File and those for Summary File     !
+-------------------------------------------------------------------------+
1                  Horiz. plot-grid start
31                 Horiz. plot-grid end
1                  Vertical plot-grid start
31                 Vertical plot-grid end
20                 Frequency of iterations to save for plotting
F                  Save some of the following fields for plotting
T  T               U velocity - u(i,j)      [ 1st col. Plot, 2nd column Summary ]
F  T               V velocity - v(i,j)
T  T               W velocity - w(i,j)
F  F               Pressure - p(i,j)
T  T               Turbulence Energy - te(i,j)
T  T               Energy dissipation rate - ed(i,j)
F  F               Effective viscosity - vis(i,j)
F  F               Mass source into gas phase - spm(i,j)
T  T               Unburnt coal passing through - colmas(i,j)
F  F               Enthalpy source into gas phase - sph(i,j)
F  F               Oxygen source into gas phase - spox(i,j)
F  T               Volatile source into gas phase - spf01(i,j)
F  F               CO source into gas phase - spco(i,j)
F  F               CO2 source into gas phase - spf02(i,j)
T  T               Mass fraction of oxygen - amox(i,j)
T  T               Mass fraction of volatiles - f01(i,j)
F  F               Mass fraction of CO - co(i,j)
T  T               Mass fraction of CO2 - f02(i,j)
T  T               (Particle temperature)**4 - stp4(i,j)
F  F               SKP (=projtd part area/unit vol.)- skp(i,j)
T  F               Radiation source in enthalpy - surad(i,j)
F  F               (Radiation temperature)**4 - tr4(i,j)
F  F               Enthalpy - h(i,j)
T  T               Temperature deg.K - t(i,j)
F  F               Density of fluid - den(i,j)
+------------------------------------------------------------ Version 2.0 --+
!                 Parameters Describing Air Input                           !
+-------------------------------------------------------------------------+
1.176              DENSIT density of air at 300 deg.K
3.6E-05            VISCOS dynamic viscosity of air at 300K in kg/ms
0.70063            SWN    swirl number over region of w velocity
9.23714            UIN    U velocity at inlet of domain in m/s
1.02397E-01        PAFIN  primary air flow kg/s
5.1325E-02         SAFIN  secondary air flow kg/s
362.16             TAIRP  primary air temperature in deg. K
389.66             TAIRS  secondary air temperature in deg. K
0.02               C11    constant for turbulence in KE model
1000.0             TEMPIN Initial gas field temperature in deg. K
+------------------------------------------------------------ Version 2.0 --+
!                  Entrance Velocity Profiles                               !
+-------------------------------------------------------------------------+
0.0                U(2,1) Initial U velocity. U(2,1),U(2,2),U(2,3),...
23.61              U(2,2)
24.97              U(2,3)
24.66              U(2,4)
20.68              U(2,5)
16.23              U(2,6)
12.48              U(2,7)
8.90               U(2,8)
4.63               U(2,9)
3.11               U(2,10)
4.3                U(2,11)
5.26               U(2,12)
6.02               U(2,13)
```

```
 6.00              U(2,14)
 -9999             End of U-velocity data
 0.0               V(1,1) Initial V velocity. V(1,1),V(1,2),V(1,3),...
 1.67              V(1,2)
 2.24              V(1,3)
 5.7               V(1,4)
 3.16              V(1,5)
 3.03              V(1,6)
 2.26              V(1,7)
 2.17              V(1,8)
 0.63              V(1,9)
 -0.57             V(1,10)
 -0.12             V(1,11)
 0.20              V(1,12)
 0.50              V(1,13)
 0.31              V(1,14)
 -9999             End of V-velocity data
 0.0               W(1,1) Initial W velocity. W(1,1),W(1,2),W(1,3),...
 0.0               W(1,2)
 0.0               W(1,3)
 0.0               W(1,4)
 0.0               W(1,5)
 0.0               W(1,6)
 0.0               W(1,7)
 0.0               W(1,8)
 0.0               W(1,9)
 2.54              W(1,10)
 3.98              W(1,11)
 4.55              W(1,12)
 4.58              W(1,13)
 4.3               W(1,14)
 -9999             End of W-velocity data
+------------------------------------------------------------- Version 2.0 -+
!                Turbulent Kinetic Energy Entrance Profile                  !
+---------------------------------------------------------------------------+
 0.00000           TE(1,1)
 1.12044           TE(1,2)
 1.25704           TE(1,3)
 1.28121           TE(1,4)
 0.87530           TE(1,5)
 0.54519           TE(1,6)
 0.32172           TE(1,7)
 0.16784           TE(1,8)
 0.04367           TE(1,9)
 0.82243           TE(1,10)
 1.71724           TE(1,11)
 2.42051           TE(1,12)
 2.87334           TE(1,13)
 2.72931           TE(1,14)
 -9999             End of Turbulent Kinetic Energy Entrance Profile data
+------------------------------------------------------------- Version 2.0 -+
!                Dissipation Entrance Profile                               !
+---------------------------------------------------------------------------+
   0.00000         ED(1,1)
  41.48298         ED(1,2)
  49.29558         ED(1,3)
  50.72441         ED(1,4)
  28.64299         ED(1,5)
  14.08007         ED(1,6)
   6.38256         ED(1,7)
   2.40503         ED(1,8)
   0.31917         ED(1,9)
  87.08052         ED(1,10)
 262.73571         ED(1,11)
 439.67481         ED(1,12)
 568.66060         ED(1,13)
 526.44223         ED(1,14)
 -9999             End of Dissipation Entrance Profile data
+------------------------------------------------------------- Version 2.0 -+
```

!	Geometry Of Furnace	!
2	ISTEP	I index of entrance plane
3	JSTEP	J index of entrance plane
31	NI	max. value of I index
31	NJ	max. value of J index
51	IT	max. value of I index
37	JT	max. value of J index
30	JOUT	location of furnace exit radius
17	IADIAB	location of end of adiabatic wall
-9999	TADIAB	wall temp. in the adiab. section. -9999=use default
410.0	TWALL	wall temperature after the adiabatic section
1	J1STP	J Grid Before Radius of Cone if no Cone set to 1
9	J2STP	J Grid Before Radius of Primary Pipe
9	J3STP	J Grid Before Radius of Second Pipe I.D.
14	J4STP	J Grid Before Radius of Second Pipe O.D.
15	J5STP	J Grid Before Radius of Quarl Start
30	J6STP	J Grid Before Radius of Adiab Wall
0.4925	RLARGE	radius of tunnel furnace in meters
5.5	ALTOT	Total Length of Furnace
2	ISTEPS	I Grid Before Start of Quarl
2	ISTEPE	I Grid Before End of Quarl
30	JSTEPE	J Grid Before Radius of O.D. of Quarl
		Version 2.0
!	X-Y Grid Locations	!
-0.015	X(1)	Axial grid coordinates X(1),...,X(31)
0.015	X(2)	
0.045	X(3)	
0.0815	X(4)	
0.1205	X(5)	
0.164	X(6)	
0.2125	X(7)	
0.2665	X(8)	
0.3265	X(9)	
0.393	X(10)	
0.467	X(11)	
0.549	X(12)	
0.640	X(13)	
0.7415	X(14)	
0.8545	X(15)	
0.980	X(16)	
1.119	X(17)	
1.274	X(18)	
1.446	X(19)	
1.637	X(20)	
1.849	X(21)	
2.085	X(22)	
2.347	X(23)	
2.639	X(24)	
2.963	X(25)	
3.323	X(26)	
3.723	X(27)	
4.175	X(28)	
4.675	X(29)	
5.225	X(30)	
5.775	X(31)	
-0.004	Y(1)	Radial grid coordinates Y(1),...,Y(31)
0.004	Y(2)	
0.012	Y(3)	
0.020	Y(4)	
0.027	Y(5)	
0.032	Y(6)	
0.036	Y(7)	
0.040	Y(8)	
0.0448	Y(9)	
0.0505	Y(10)	
0.0554	Y(11)	
0.06025	Y(12)	

```
0.066              Y(13)
0.0727             Y(14)
0.0797             Y(15)
0.08705            Y(16)
0.0958             Y(17)
0.1068             Y(18)
0.1185             Y(19)
0.1312             Y(20)
0.1468             Y(21)
0.165              Y(22)
0.186              Y(23)
0.2102             Y(24)
0.2384             Y(25)
0.2709             Y(26)
0.3085             Y(27)
0.351              Y(28)
0.4048             Y(29)
0.4632             Y(30)
0.5218             Y(31)
+------------------------------------------------------------ Version 2.0 --------+
!                  End of the MODTUN Input Parameter File                          !
+------------------------------------------------------------------------------+
```

Appendix J FAFNIR Input Parameter File

```
+------------------------------------------------------------- Version 4.1 ----+
!                      FAFNIR Parameter File          (in house version 5.0)  !
+-----------------------------------------------------------------------------+
C1 IEA TestCase : Case D; Grid after Lockwood
C2 Run: 7-500 combustion run with GIBBS, IQUICK ON, URTRAK=.05, Kg=.5
C3           decrease Harwell pre-expo. for devol. by half
C4      8-3000 continue run#7
C5      9-5   repeat converged run#8 to print out more variables
C6+-----------------------------------------------------------------------------+
C7!  New Parameters, July 18 1991 : URTRAK, AKGCINIT, ETWALL, EOWALL, EWWALL  !
C8+-----------------------------------------------------------------------------+
C9
+------------------------------------------------------------- Version 4.1 ----+
!                     Fundamental Parameters                                  !
+-----------------------------------------------------------------------------+
5                   MAXIT   number of iterations in the current run
51                  NI      axial dimension of the simulation grid
37                  NJ      radial dimension of the simulation grid
12                  IMON    axial index of monitoring location
12                  JMON    radial index of monitoring location
2                   NINL    number of inlets (max. 10)
6                   NTH     number of polar directions for angular grid
4                   NFI     number of azimuthal directions for ang grid
3.00E-3             SORMAX  maximum sum of sources
+------------------------------------------------------------- Version 4.1 ----+
!                     I/O Control                                             !
+-----------------------------------------------------------------------------+
T                   IREAD   T - read initial field data, F - start at iteration 1
T                   IWRITE  T-full output at MAXIT, F-reduced outp on nonconverg.
T                   IWSORC  print all sources of partic. phase given to gas phase
1                   IPRESD  print the residuals every this many iterations
T                   INCALC  T-run FAFNIR,  F-just print INIT.DAT
F                   INOUT   print the initial field
T                   ECHO    echo the input parameters in a file called ECHO.OUT
5                   PHFREQ full particle histories every this many iterations
1 2 3 4 5 6 7 8 9 10<--- Starting location indecies (columns)
F F F F F F F F F F 1
F F T F F F F F F F 2
F F F F F F F F F F 3       +-----------------------------------------+
T F F F F F F F F F 4       ! PPHIST - Particle history output matrix !
F F F F F F F F F F 5       +-----------------------------------------+
F F F F F F F F F F 6
F F F F F F F F F F 7    PPHIST(i,j) - TRUE means full output for particle
F F F F F F F F F F 8                  size i at starting location j.
F F F F F F F F F F 9
F F F F F F F F F F 10<--- Particle size indecies (rows)
+------------------------------------------------------------- Version 4.1 ----+
!                     Entrance profile and grid control                       !
+-----------------------------------------------------------------------------+
2                   UPROF  1 - uniform, 2 - explicit, 3 - mass flow
2                   VPROF  1 - uniform, 2 - explicit
2                   WPROF  1 - uniform, 2-explicit, 3-swirl number,4-swirl angle
2                   TKEPROF (Turb.K.E.)   1 - default, 2 - explicit
2                   DISPROF (Dissipation) 1 - default, 2 - explicit
2                   XYGRID 1 - default, 2 - explicit, 3 - AUTOGR subroutine
+------------------------------------------------------------- Version 4.1 ----+
!                          Final Plot Data Generation                         !
+-----------------------------------------------------------------------------+
F                   Generate final plot-data for the following parameters:
T                   U velocity - u(i,j)
F                   V velocity - v(i,j)
T                   W velocity - w(i,j)
F                   Pressure - p(i,j)
T                   Turbulence Energy - te(i,j)
T                   Energy dissipation rate - ed(i,j)
F                   Effective viscosity - vis(i,j)
```

```
F                Mass source into gas phase - spm(i,j)
F                Enthalpy source into gas phase - sph(i,j)
F                Oxygen source into gas phase - spox(i,j)
F                Volatile source into gas phase - spfvol(i,j)
T                Mass fraction of oxygen - amox(i,j)
T                Mass fraction of volatiles - fvol(i,j)
T                (Particle temperature)**4 - stp4(i,j)
F                SKP (=projtd part area/unit vol.)- skp(i,j)
T                Radiation source in enthalpy - surad(i,j)
F                (Radiation temperature)**4 - tr4(i,j)
F                Enthalpy - h(i,j)
T                Temperature deg.K - t(i,j)
F                Density of fluid - den(i,j)
F                Radiation intensity source function - ra(i,j)
+------------------------------------------------------------ Version 4.1 ---+
!            Plot data generation for convergence monitoring                  !
+-----------------------------------------------------------------------------+
F                Generate convergence-test plot data
2                Generate convergence-test plot data every this many iteratns.
12               X1 axial grid-coordinate of convergence-test point #1
12               Y1 radial grid-coordinate of convergence-test point #1
1                X2 axial grid-coordinate of convergence-test point #2
19               Y2 radial grid-coordinate of convergence-test point #2
+------------------------------------------------------------ Version 4.1 ---+
!            Parameters To Control Convergence                                !
+-----------------------------------------------------------------------------+
3                NSWPU   # of sweeps for U
3                NSWPV           "       V
2                NSWPW           "       W
1                NSWPP           "       P
2                NSWPK           "       K
2                NSWPD           "       D
5                NSWPX           "       X
2                NSWPH           "       H
2                NSWPVO          "       VO
2                NSWPPR          "       PR
5                NSWPRA          "       RA
35               MAXSWP # of sweeps for P if PISO is used and NSWPP=1
0.20             RESF   sweep until residual ratio < RESF or MAXSWP is reached
1                MAXSRA # of sweeps for the intensity loop
0.01             RESRA  sweep until change in wall radiant flux < RESRA
0.65             URFU   under relaxation factor for U
0.65             URFV                    "               V
0.60             URFW                    "               W
1.0              URFP                    "               P
0.5              URFK                    "               K
0.5              URFE                    "               E
1.0              URFVIS                  "             VIS
0.5              URFX                    "               X
0.5              URFVOL                  "             VOL
0.2              URFDEN                  "             DEN
0.5              URFH                    "               H
0.5              URFPR                   "              PR
1.0              URFTEM                  "             TEM
1.0              URFRAD                  "             RAD
0.05             URTRAK                  "       particle tracking [New Jul '91]
+------------------------------------------------------------ Version 4.1 -+
!                  Computation Control Parameters                           !
+-----------------------------------------------------------------------------+
T                INCALU Calculate u-velocity
T                INCALV    "      v-velocity
T                INCALW    "      w-velocity
T                INCALP    "      pressure
T                INCALK    "      turbulent kinetic energy
T                INCALD    "      dissipation
T                INCALH    "      enthalpy
T                INCALT    "      temperature
T                INCARD    "      radiation
T                INCALX    "      oxygen
```

```
T                 INCAVO    "      volatile
T                 INCAPR    "      product
T                 INPRO  Enable the call to the properties routine
T                 IPISO  T-use PISO algorithm on Pressure eq. F-use SIMPLE alg.
F                 ISIMC  simult. devolatilisation and char combustion
T                 IQUICK Use the quick discretization scheme
F                 INCAIN Use the Finite Volume Method for radiation
10                INFREQ Use the FV method every this many iteration
+------------------------------------------------------------ Version 4.1 -----+
!                 Coal Related Quantities                                      !
+-----------------------------------------------------------------------------+
1                 INLCOL coal inlet number
0.01403           COLFLO coal mass flow rate (kg/s)
1512.6            DENPO  initial coal density (kg/m**3)
0.2560            FRESC % of C in coal
0.4417            FVOLC % of volatiles if coal
0.0379            FHY    mass fraction of hydrogen in coal
0.0026            FSU    % of S in coal
0.0093            FN2    % of N2 in coal
0.1515            FOX    % of O2 in coal
0.0               FH2O   mass fraction of H2O in coal
0.1010            FASH   % of ash in coal
328.10E+05        CALVAL calorific value of carbon (J/kg)
0.4940E+08        ACTEV  activation energy for devolatilisation (J/kmol)
1.0000E+05        FKSO   pre-expon. factor for devolatilisation (1/s)
0.854E+08         ACTEK  activation energy for char combustion (J/kmol)
1.301E-02         AFFACT pre-expon. factor for char combustion (kg/m^2sPa)
6.279E+05         HVOLEP latent heat of volatile evaporation (J/kg)
4.0               ACOMB
2.0               BCOMB
+------------------------------------------------------------ Version 4.1 ---+
!                Particle Tracking Parameters                                 !
+-----------------------------------------------------------------------------+
T                 ITRACK enable the particle tracking routines
1                 INTRAK calculate particle tracking every this many iterations
1                 ITRAK1 starting iteration number for particle tracking
T                 ICOMB  enable particle combustion calculation
F                 NOSLIP disable the drag law effect in trajectory calculation
4                 NPS    # of particle sizes to be tracked (max = 10)
1.2E-05           PD(1)   particle diameter
3.80E-05          PD(2)
6.2E-05           PD(3)
8.80E-05          PD(4)
0.180             FRACT(1) fraction of particles in particle size
0.250             FRACT(2)
0.210             FRACT(3)
0.360             FRACT(4)
4                 NSL     # of particle starting locations (max = 10)
0.0100            YST(1)  distance of firing location of particle
0.0190            YST(2)  from center in m
0.0290            YST(3)
0.0380            YST(4)
28.94             UPST(1) particle start velocity in m/s
29.15             UPST(2)
22.33             UPST(3)
12.46             UPST(4)
+------------------------------------------------------------ Version 4.1 --+
!                  Fluid Properties                                          !
+-----------------------------------------------------------------------------+
3.6E-5            VISCOS  Laminar viscosity (Ns/m**2)
0.5               SCHMDT  Schmidt number
0.9               PRANDT  Prandtl number
0.09              CMU     Turbulence model constants *check*
1.0               CT *check*
1.44              C1 *check*
1.92              C2 *check*
1.00              TURINT  Turbulent Intensity in inlet and initial turb. calc.
0.005             ALAMDA  Length scale for initial and inlet dissipation
0.23              OXIN(1) oxygen concentration at inlet #1 *NEW*
```

```
0.23              OXIN(2) oxygen concentration at inlet #2 *NEW*
0.0               PREF    Pressure of reference (Pa)
300               TREF    Temperature of reference (deg.K)
2                 IPREF   axial grid coordinate of the reference point
2                 JPREF   radial grid coordinate of the reference point
1.176             DENSIT  (kg/m^3)
0.4187            CAPPA   *NEW*
9.793             ELOG    *NEW*
0.5               PRH     *NEW*
1.0               PRTE    *NEW*
1.0               PRED    *NEW*
0.7               PRLAM   *NEW*
0.5               ETWALL  Emmissivity (TOP)  [ New Jul '91 ]
0.8               EOWALL  Emmissivity        [ New Jul '91 ]
1.0               EWWALL  Emmissivity (WEST) [ New Jul '91 ]
0.5               AKGCINIT  Gas absorption coefficient  [ New Jul '91 ]
+------------------------------------------------------------ Version 4.1 -->+
!                  U Velocity Entrance Profile                               !
+------------------------------------------------------------------------------+
24.000            UINL(1) U velocity at inlet #1
5.000             UINL(2) U velocity at inlet #2
1.02397E-01       FLOINL(1) Mass flow at inlet #1 (kg/s)
5.1325E-02        FLOINL(2) Mass flow at inlet #2 (kg/s)
0.000             UIN(1) Explicit initial U velocity
27.1000           UIN(2)
28.4300           UIN(3)
29.5000           UIN(4)
28.5600           UIN(5)
23.2600           UIN(6)
16.7400           UIN(7)
12.460            UIN(8)
8.470             UIN(9)
3.020             UIN(10)
4.050             UIN(11)
5.640             UIN(12)
6.200             UIN(13)
-9999             End of explicit U-velocity data
+------------------------------------------------------------ Version 4.1 -->+
!                  V Velocity Entrance Profile                               !
+------------------------------------------------------------------------------+
3.5               VINL(1) V velocity at inlet #1
0.000             VINL(2) V velocity at inlet #2
0.0               VIN(1)  Explicit initial V velocity
1.56              VIN(2)
1.83              VIN(3)
2.50              VIN(4)
3.12              VIN(5)
3.17              VIN(6)
3.65              VIN(7)
3.09              VIN(8)
2.46              VIN(9)
0.91              VIN(10)
-0.47             VIN(11)
0.05              VIN(12)
0.56              VIN(13)
-9999             End of explicit V-velocity data
+------------------------------------------------------------ Version 4.1 -->+
!                  W Velocity Entrance Profile                               !
+------------------------------------------------------------------------------+
0.00              WINL(1) W velocity at inlet #1
4.00              WINL(2) W velocity at inlet #2
2                 INLSW   The number of the inlet with the swirl
0.70              SWNUMB  Swirl number at inlet INLSW
60.0              SWANGL  Swirl angle (in degrees) at inlet INLSW
0.0               WIN(1) Explicit initial W velocity
0.0               WIN(2)
0.0               WIN(3)
0.0               WIN(4)
0.0               WIN(5)
```

```
0.0             WIN(6)
0.0             WIN(7)
0.0             WIN(8)
0.30            WIN(9)
1.67            WIN(10)
5.18            WIN(11)
6.44            WIN(12)
6.09            WIN(13)
-9999           End of explicit W-velocity data
+------------------------------------------------------------- Version 4.1 -+
!              Turbulent Kinetic Energy Entrance Profile                     !
+----------------------------------------------------------------------------+
0.00000         TE(1,1)
1.47369         TE(1,2)
1.62323         TE(1,3)
1.75300         TE(1,4)
1.65082         TE(1,5)
1.10215         TE(1,6)
0.58710         TE(1,7)
0.32960         TE(1,8)
3.89413         TE(1,9)
0.63687         TE(1,10)
2.17279         TE(1,11)
3.66429         TE(1,12)
3.79209         TE(1,13)
-9999           End of Turbulent Kinetic Energy Entrance Profile data
+------------------------------------------------------------- Version 4.1 -+
!                     Dissipation Entrance Profile                           !
+----------------------------------------------------------------------------+
0.00000         ED(1,1)
62.57399        ED(1,2)
72.33609        ED(1,3)
81.18181        ED(1,4)
74.18804        ED(1,5)
40.47144        ED(1,6)
15.73455        ED(1,7)
6.61859         ED(1,8)
897.19624       ED(1,9)
59.34017        ED(1,10)
373.93769       ED(1,11)
818.94829       ED(1,12)
862.16365       ED(1,13)
-9999           End of Dissipation Entrance Profile data
+------------------------------------------------------------- Version 4.1 -+
!                     Furnace Geometry                                       !
+----------------------------------------------------------------------------+
0.4925          RLARGE  radius of tunnel furnace in meters
5.37            ALTOT   total length of the calculation domain
2               IINL    index of the inlet plane
1               JINL(1) J Grid before start of inlet #1
10              JINL(2) J Grid before O.D. of inlet #1
10              JINL(3) J Grid before start of inlet #2
13              JINL(4) J Grid before O.D. of inlet #2
Primary         INLNAM(1) name of inlet 1
Secondary       INLNAM(2) name of inlet 2
T               IQUARL  T - a quarl exists
T               IEXPAN  T - a step exists
32              ISTEP   I index just before the wall (step) intersection
34              JSTEP   J index just before the wall (step) intersection
15              IQRL1   I index of quarl start
25              IQRL2   I index of quarl end
15              JQRL1   J index of quarl start
25              JQRL2   J index of quarl end
29              JOUT    location of the outlet wall (use NI-1 if no outwall)
+------------------------------------------------------------- Version 4.1 -+
!                     Temperatures                                           !
+----------------------------------------------------------------------------+
362.16          TIN(1)  temperature at inlet #1
389.66          TIN(2)  temperature at inlet #2
```

```
1000.0              TAIR    initial air temperature (deg.K)
F                   INITT   initialize entire field temp. to the air temperature
T                   INTERWT use interpolation to compute TWALL(1)..TWALL(NI)
353.0     -0.1      Dummy
353.0     1.24      TWALL(1) / axial dist.for the 1st interpolation point *NEW*
353.0     1.39      TWALL(2) / axial dist.for the 2nd interpolation point *NEW*
353.0     1.54      TWALL(3)  Temperatures are in deg. K.
353.0     1.68      TWALL(4)
353.0     1.84      TWALL(5)
353.0     5.40      TWALL(6)
-9999               End of wall temperature data.
+------------------------------------------------------------- Version 4.1 -+
!                   Adiabatic wall specifications                           !
+---------------------------------------------------------------------------+
1                   Start of the 1st adiabatic region
32                  End of the 1st adiabatic region
-9999                Start of the 2nd adiabatic region  [-9999 means that there
-9999                End of the 2nd adiabatic region     is no adiab. region ]
+------------------------------------------------------------- Version 4.1 -+
!              X-Y grid generation using the AUTOGR subroutine              !
+---------------------------------------------------------------------------+
7                   IA  x start index
0.055               XA  x coordinate at start
29                  IB  x end index
3.0                 XB  x coordinate at the end
1.2                 EPS expansion factor for x
7                   JA  y start index
0.055               YA  y coordinate at start
29                  JB  y end index
3.0                 YB  y coordinate at the end
+------------------------------------------------------------- Version 4.1 -+
!                      Explicit X-Y grid                                    !
+---------------------------------------------------------------------------+
-0.005              X(1)     Axial grid coordinates X(1),...,X(51)
0.005               X(2)
0.0160              X(3)
0.0280              X(4)
0.0410              X(5)
0.0550              X(6)
0.0700              X(7)
0.086               X(8)
0.103               X(9)
0.120               X(10)
0.1364              X(11)
0.1564              X(12)
0.1764              X(13)
0.1964              X(14)
0.2164              X(15)
0.2364              X(16)
0.2564              X(17)
0.2755              X(18)
0.2955              X(19)
0.3150              X(20)
0.3335              X(21)
0.3530              X(22)
0.369               X(23)
0.390               X(24)
0.4125              X(25)
0.4299              X(26)
0.530               X(27)
0.630               X(28)
0.73                X(29)
0.84                X(30)
0.96                X(31)
1.09                X(32)
1.21                X(33)
1.32                X(34)
1.43                X(35)
1.60                X(36)
```

```
1.85              X(37)
2.05              X(38)
2.30              X(39)
2.60              X(40)
2.90              X(41)
3.20              X(42)
3.50              X(43)
3.80              X(44)
4.10              X(45)
4.40              X(46)
4.65              X(47)
4.90              X(48)
5.10              X(49)
5.25              X(50)
5.40              X(51)
-0.002            Y(1)   Radial grid coordinates  Y(1),...,Y(37)
0.002             Y(2)
0.0070            Y(3)
0.014             Y(4)
0.021             Y(5)
0.0280            Y(6)
0.03372           Y(7)
0.03772           Y(8)
0.04172           Y(9)
0.04560           Y(10)
0.04970           Y(11)
0.0610            Y(12)
0.0717            Y(13)
0.0807            Y(14)
0.0877            Y(15)
0.0965            Y(16)
0.1061            Y(17)
0.1156            Y(18)
0.1249            Y(19)
0.1341            Y(20)
0.1433            Y(21)
0.1520            Y(22)
0.1600            Y(23)
0.1700            Y(24)
0.1803            Y(25)
0.1888            Y(26)
0.20              Y(27)
0.215             Y(28)
0.235             Y(29)
0.260             Y(30)
0.290             Y(31)
0.325             Y(32)
0.365             Y(33)
0.400             Y(34)
0.434             Y(35)
0.475             Y(36)
0.5093            Y(37)
+------------------------------------------------------- Version 4.1 --------+
!                 End of the MODTUN Input Parameter File                      !
+-------------------------------------------------------------------------------+
```